The Exact Ground State of the Frenkel-Kontorova Model with Repeated Parabolic Potential
I. Basic Results

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The problem of finding the exact energies and configurations for the Frenkel-Kontorova model consisting of particles in one dimension connected to their nearest-neighbors by springs and placed in a periodic potential consisting of segments from parabolas of identical (positive) curvature but arbitrary height and spacing, is reduced to that of minimizing a certain convex function defined on a finite simplex.

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I. INTRODUCTION

The Frenkel-Kontorova model of classical particles connected to their nearest neighbors by springs and placed in a one-dimensional periodic potential V [1–4] is of interest for several different reasons. First, it provides a simple example which exhibits some of the complex phenomena (discommensurations, devil's staircase phase diagrams) associated with commensurate-incommensurate phase transitions [5]. For some recent studies, see [6,7]; also [8] for extensions to quantum systems, and [9] for classical particles at a finite temperature. Next, various interesting dynamical phenomena result if forces, either static or dynamic, are applied to the particles in a Frenkel-Kontorova chain; for some recent work, see [10,11]. Finally, the equilibrium configurations of this model form the orbits of an area-preserving twist map [12], so that their study is part of the subject of nonlinear dynamical systems [13].

A special, exactly solvable realization introduced by Aubry [14] and Percival [15], in which V consists of a potential made up of identical parabolas, has played a pioneering role in the study of general Frenkel-Kontorova models. It is particularly useful for understanding the properties of incommensurate ground states in the "Cantorus" regime: such configurations define invariant Cantor sets of the associated area-preserving map, on which the motion is quasiperiodic with an irrational winding number w. Cantori, or Aubry-Mather sets [16], have been the subject of considerable research [17–22], as they constitute the ubiquitous remnants of broken KAM tori in non-integrable Hamiltonian systems [23].

The present paper is dedicated to a generalization of this solvable model to the case in which the parabolas all have the same curvature, but need not be uniformly spaced nor located at the same height. The only constraint is that after N parabolas, where N is finite, the whole pattern is repeated, thus giving rise to a periodic V. See the example with $N = 3$ sketched in Fig. 1. The case $N = 1$ is, of course, the one studied earlier by Aubry and Percival.

The generalization is important for two reasons: First, as we pointed out for $N = 2$ in a previous paper [24], qualitatively novel phenomena emerge which are not present in the case $N = 1$. Examples are incommensurate defects, discontinuous Cantorus-Cantorus phase transitions, and independent orbits of gaps composing the complement of the Aubry-Mather set. Second, it provides a tool, through the possibility of

approximating a smooth potential by a set of parabolas, for identifying true ground states in the presence of infinite sets of competing metastable Cantorus configurations, as encountered in Frenkel-Kontorova models with smooth V differing from a simple cosine [25].

In the following sections we give the detailed solution for general N, which in essence consists in replacing the original infinite-variable minimization problem by that of finding the minimum of a certain convex function defined on a finite simplex. While the second minimization problem is not altogether trivial, it can be carried out to quite adequate precision in particular cases by a combination of analytical and numerical techniques. Efficient numerical methods are the subject of the paper which follows.

Previous research on this topic of which we are aware includes an unpublished thesis of F. Vallet [26]. He considered some particular cases for $N > 1$, including the $N = 2$ situation with equally spaced parabolas discussed in our previous publication, for which he wrote down an explicit expression for the ground state energy. And he pointed out that the same methods could be applied to the general N situation using a parametrization of the hull function very similar to the one employed here. More recently Kao, Lee, and Tzeng [27] have addressed the problem of finding the ground state by using a hull function to find solutions of the equilibrium equations. Their results are consistent with those in the present manuscript.

In addition, Aubry, Axel and Vallet considered a somewhat different extension of the $N = 1$ solvable model, with even and odd numbered particles subjected to different potentials [28]. While there are certain similarities, this model (and the method used to solve it) seems to be distinct from the $N = 2$ case considered here. Recently Kao, Lee, and Tzeng [29] have solved a model in which the parabolas have negative curvature; the results are very different from the case of positive curvature discussed here.

Our material is organized as follows. Section II contains basic definitions for the model including the explicit form of the potential V. In Sec. III the energy for an equilibrium state is rewritten with the help of a Green's function in a form which is combined with some of Aubry's exact results for ground states in Sec. IV. The result is used in Sec. V to set up an explicit minimization problem of a convex function over a finite simplex, the solution to which yields both the energy and configuration of the ground state. The conclusion, Sec. VI, indicates a number of possible generalizations. Minor technical issues are discussed in two appendices.

II. ENERGY

We shall consider a system described by an energy

$$H = \sum_{j=-\infty}^{\infty} [\frac{1}{2}(u_{j+1} - u_j)^2 + V(u_j)], \tag{2.1}$$

where u_j is the position of the j-th particle, while

$$V(u) = V(u + P) = \min_n p(n; u) \tag{2.2}$$

is a periodic potential made up of segments of parabolas, as illustrated by Fig. 1. The n-th parabola is given by the formula

$$p(n; u) = \frac{1}{2}\kappa(u - t_n)^2 + h_n. \tag{2.3}$$

We assume that the positions of the minima of these parabolas form a monotonic periodic sequence,

$$t_n < t_{n+1} ; \quad t_{n+N} = P + t_n \tag{2.4}$$

and the values at the minima are periodic,

$$h_{n+N} = h_n, \tag{2.5}$$

but otherwise arbitrary.

Because all the parabolas have the same curvature, the u axis consists of segments separated by a sequence of *dividing points*, (see Fig. 1),

$$\bar{t}_n \leq \bar{t}_{n+1}; \quad \bar{t}_{n+N} = P + \bar{t}_n, \tag{2.6}$$

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with the property that for u in the open interval $(\bar{t}_{m-1}, \bar{t}_m)$ (which may be empty), the minimum in (2.2) is achieved for $n = m$, and for no other value of n. Thus this interval is uniquely associated with the m'th parabola, and if u_j falls in this interval, we shall say that particle j is "in" parabola m, or $n(j) = m$. Given the periodicity (2.6), it is clear that two such intervals whose subscripts differ by N will be of the same length, and will have corresponding values of $V(u)$. Thus we shall say that such an interval, or the corresponding parabola, is of "type l", $1 \le l \le N$, if $m = l \pmod{N}$.

Let

$$\tau_j = t_{n(j)} \tag{2.7}$$

be the minimum of the parabola containing the j-th particle, in the sense just discussed. Then (2.1) can be rewritten as

$$H = H_0 + H_1, \tag{2.8}$$

where

$$H_0 = \frac{1}{2} \sum_{j=-\infty}^{\infty} [(u_{j+1} - u_j)^2 + \kappa(u_j - \tau_j)^2] \tag{2.9}$$

and

$$H_1 = \sum_{j=-\infty}^{\infty} h_{n(j)}. \tag{2.10}$$

For later analysis it is convenient to rewrite (2.9) in terms of

$$\hat{u}_j = u_j - \tau_j, \tag{2.11}$$

the distance of the j-th particle from the minimum of the parabola which contains it. One obtains

$$H_0 = \frac{1}{2} \sum_{j=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} H_a(j-k)\hat{u}_j\hat{u}_k - \sum_{j=-\infty}^{\infty} \hat{u}_j \Delta^2 \tau_j + \frac{1}{2} \sum_{j=-\infty}^{\infty} (\Delta \tau_j)^2, \tag{2.12}$$

where

$$\Delta \tau_j = \tau_{j+1} - \tau_j, \quad \Delta^2 \tau_j = \tau_{j+1} - 2\tau_j + \tau_{j-1} = \Delta \tau_j - \Delta \tau_{j-1} \tag{2.13}$$

and

$$H_a(0) = 2 + \kappa, \quad H_a(1) = H_a(-1) = -1, \quad H_a(k) = 0 \text{ for } |k| > 1. \tag{2.14}$$

III. EQUILIBRIUM STATES

An equilibrium state is one in which the force is zero on every particle, which means $\partial H_0 / \partial \hat{u}_j = 0$ for every j, and thus, by (2.12),

$$\sum_{k=-\infty}^{\infty} H_a(j-k)\hat{u}_k = \Delta^2 \tau_j \tag{3.1}$$

If we assume that the $\Delta^2 \tau_j$ are known and are bounded as a function of j, the solution of (3.1) may be written as

$$\hat{u}_j = \sum_{k=-\infty}^{\infty} G(j-k)\Delta^2 \tau_k \tag{3.2}$$

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using the Green's function (decreasing at infinity)

$$G(k) = e^{-r|k|}/2\sinh r, \tag{3.3}$$

which satisfies the equation

$$\sum_{k=-\infty}^{\infty} H_a(j-k)G(k-l) = \delta_{jl}. \tag{3.4}$$

Here r is a positive number defined by:

$$\kappa = (2\sinh r/2)^2. \tag{3.5}$$

Multiplying (3.1) by $\hat{u}_j$ and summing yields, see (2.12) and (3.2):

$$H_0 - \frac{1}{2}\sum_{j=-\infty}^{\infty}(\Delta\tau_j)^2 = -\frac{1}{2}\sum_{j=-\infty}^{\infty}\hat{u}_j\Delta^2\tau_j = -\frac{1}{2}\sum_{j=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}G(j-k)\Delta^2\tau_j\Delta^2\tau_k. \tag{3.6}$$

With the help of the function

$$g(j) = G(j+1) + G(j-1) - 2G(j) + \delta_{j0} = (\tanh r/2)e^{-r|j|}. \tag{3.7}$$

one can rewrite (3.2) and (3.6) as:

$$u_j = \sum_{k=-\infty}^{\infty} g(j-k)\tau_k, \tag{3.8}$$

$$H_0 = \frac{1}{2}\sum_{j=-\infty}^{\infty}\sum_{k=-\infty}^{\infty} g(j-k)\Delta\tau_j\Delta\tau_k. \tag{3.9}$$

The fact that

$$\sum_{j=-\infty}^{\infty} g(j) = 1 \tag{3.10}$$

means that (3.8) expresses the position of particle j as a weighted average of the positions of the parabolas occupied by the different particles.

It is useful for later purposes to extend $g(j)$ to a function $g(x)$ defined on the entire real axis by means of linear interpolation between successive integers, (see Fig. 2), which is to say:

$$g(x) := [1 - \text{frac}(x)]g(\text{Int}(x)) + \text{frac}(x)g(1 + \text{Int}(x)), \tag{3.11}$$

where $\text{Int}(x)$ is the largest integer not greater than x, and $\text{frac}(x)$ stands for $x - \text{Int}(x)$. Note that the resulting function is convex for $x > 0$, and also for $x < 0$, and possesses a piecewise constant derivative with discontinuities whenever x is an integer.

If the equilibrium configuration is monotonic in the sense that for all j,

$$n(j+1) \geq n(j), \tag{3.12}$$

that is, $\Delta\tau_j \geq 0$, then one can write H_0, (3.9) in an alternative form with the help of the function,

$$I_m = \max\{j\epsilon\mathbb{Z} \mid n(j) \leq m\}, \tag{3.13}$$

the number of the last particle in parabola m, or of the last particle preceding this parabola if it is empty. (One can think of I_m as a sort of inverse of the function $n(j)$.) If

$$\Delta t_m = t_{m+1} - t_m \tag{3.14}$$

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is the distance between the minima of two successive parabolas, it is easy to show that

$$\tau_{j+1} - \tau_j = \Delta\tau_j = \sum_{m=-\infty}^{\infty} (\Delta t_m)\delta_{j,I_m}. \tag{3.15}$$

Thus if particle j is not the last particle in some parabola, which is to say particle $j + 1$ is in the same parabola, I_m never takes the value j and $\Delta\tau_j = 0$, so both sides of this equation vanish. If j is the last particle in parabola m and parabola $m + 1$ is not empty, then $\Delta\tau_j = \Delta t_m$, $I_m = j$, and I_{m+1} is larger than j, so again (3.15) holds. If, on the other hand, parabola m is followed by one or more empty parabolas, then for each of these I takes the same value j, and thus $\Delta\tau_j$ is expressed as the correct sum of Δt intervals. With the help of (3.15), (3.9) can be written as

$$H_0 = \frac{1}{2} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} g(I_n - I_m)\Delta t_m \Delta t_n \tag{3.16}$$

with sums over parabolas instead of particles. Similarly (2.10) may be written in the form

$$H_1 = \sum_{m=-\infty}^{\infty} (I_m - I_{m-1})h_m, \tag{3.17}$$

because $I_m - I_{m-1}$ is equal to the number of particles in parabola m.

IV. CONTRIBUTION OF H_0 TO THE GROUND STATE ENERGY

For an infinite configuration $\{u_j\}_{j\epsilon\mathbb{Z}}$ of particles, expressions such as (2.1) are formally infinite and do not possess a direct interpretation. Following Aubry [30], we shall understand (2.1) as prescribing the change in energy if any finite set of particles are displaced from one set of positions to another. A *minimum energy configuration* is one for which any such change increases H (or leaves it constant) and a *ground state* is a minimum energy configuration which satisfies certain recurrence conditions [30]. Aubry has shown that under suitable conditions (see also the additional remarks in App. A) any minimum energy configuration has a well-defined average separation between particles,

$$\omega = Pw := \lim_{(k-j)\to\infty} (u_k - u_j)/(k - j), \tag{4.1}$$

independent of how j and k behave individually (thus $j = -k$, or $j = k/2$ give the same result when $k \to \infty$). We shall call $w = \omega/P$ the "winding number", a notation clearly motivated by the twist map analogy [13].

For a given ω, there is a well-defined energy per particle

$$\epsilon = \lim_{(K-J)\to\infty} \frac{1}{(K - J)} \sum_{j=J}^{K-1} [\frac{1}{2}(u_{j+1} - u_j)^2 + V(u_j)], \tag{4.2}$$

where $\{u_j\}$ is any minimum energy configuration for this ω. (Note that this is different from the process of choosing, for each J and K fixed, the $\{u_j\}$ which minimizes the finite sum in (4.2) !)

If w is irrational, any ground state configuration with $\omega = Pw$ has the form

$$u_j = f_\omega(j\omega + c), \tag{4.3}$$

where c is some constant, and $f_\omega(z)$ is a monotone strictly increasing "hull" function [30] which is step periodic, i.e.,

$$f_\omega(z + P) = P + f_\omega(z). \tag{4.4}$$

When f_ω is discontinuous, as it is for the $V(u)$ considered here, the discontinuities form a dense set, and there are two versions of f_ω: f_ω^+, which at each discontinuity takes the maximum possible value consistent with monotonicity, and is thus right-continuous, or upper semi-continuous, or f_ω^-, which takes the minimal

possible value at each discontinuity, and is thus left continuous, or lower semi-continuous. Either f_ω^+ or f_ω^- may be employed in (4.3), though not both simultaneously [30].

When $w = p/q$ is rational, with p and q relatively prime integers and $q > 0$, one can again write ground state configurations in the form (4.3), where the function $f_\omega(z)$ is defined on the discrete set of points $z = Ps/q$, where s is any integer, and c is an integer multiple of P/q. Defined in this way, $f_\omega(z)$ is strictly increasing and satisfies (4.4). See App. B for the derivation of this result, which does not seem to be explicitly stated in [30]. For convenience of exposition, we shall assume that w is irrational in the following discussion, as the extension to the case of rational w is straightforward.

In a ground state configuration no u_j can come closer than some fixed finite distance to one of the dividing points $\bar{t}_n$, (2.6) (see App. A). Hence $f_\omega(z)$ will have jump discontinuities with every $\bar{t}_n$ falling in the interior of one of these discontinuities, as illustrated in Fig. 3. As $f_\omega(z)$ is monotone, this means that the z axis is cut up into segments by dividing points

$$\bar{z}_n \leq \bar{z}_{n+1}; \quad \bar{z}_{n+N} = \bar{z}_n + P \tag{4.5}$$

with the property that

$$z < \bar{z}_n < z' \;\Rightarrow\; f_\omega(z) < \bar{t}_n < f_\omega(z'). \tag{4.6}$$

Thus there is a correspondence between intervals on the z axis and those on the u axis in that $(\bar{z}_{n-1}, \bar{z}_n)$ is mapped by f_ω into the interior of $(\bar{t}_{n-1}, \bar{t}_n)$, so that intervals of type l on one axis correspond to intervals of type l on the other.

The preceding discussion allows us to find an explicit formula for the integers $\{I_m\}$ defined in (3.13) in terms of the $\bar{z}_m$. Assume the hull function is f_ω^-. Then, see Fig. 3, the number of the last particle falling in parabola m (or preceding this parabola if it is empty) is the largest integer j for which

$$j\omega + c \leq \bar{z}_m, \tag{4.7}$$

which means

$$I_m = \text{Int}[(\bar{z}_m - c)/\omega]. \tag{4.8}$$

(If one employs f_ω^+ rather than f_ω^-, (4.7) is a strict inequality, and Int in (4.8) should be replaced by int, where $\text{int}(x)$ is the largest integer strictly less than x. The energy per particle is independent of the choice between f_ω^+ and f_ω^-.)

The ground state energy per particle ϵ_0 corresponding to H_0, (3.16), can be computed as follows: Consider a set of LN successive parabolas, where L is large. Suppose that two integers m_0, n_0 between 1 and N are given, and consider summands in (3.16) corresponding to pairs

$$(m, n) = (m_0 + \mu N, n_0 + (\mu + \nu)N), \tag{4.9}$$

where μ and ν are integers, and μ is between 1 and L. By (2.4), Δt_m and Δt_n are the same for all m and n of this type, while (4.5), the step periodicity of the $\bar{z}_n$, allows us to write

$$I_n - I_m = \text{Int}(D + A + \mu/w) - \text{Int}(A + \mu/w), \tag{4.10}$$

where w is ω/P,

$$A = \zeta_{m_0}/w - c/\omega, \quad D = (\zeta_{n_0} - \zeta_{m_0} + \nu)/w, \tag{4.11}$$

and we have introduced the notation

$$\zeta_n := \bar{z}_n/P. \tag{4.12}$$

As μ varies, the right side of (4.10) takes on only two values: $1 + \text{Int}(D)$, which occurs for a fraction $\text{frac}(D)$ of the values of μ, assuming w is irrational and L is very large, and $\text{Int}(D)$, which occurs for a fraction $1 - \text{frac}(D)$ of the μ values. Hence the sum of $g(I_n - I_m)$ over the pairs (4.9) with ν fixed is for large L given by $Lg(D)$, using the extended definition of g in (3.11).

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What remains is a sum over ν, which can be extended from $-\infty$ to ∞ with negligible error because g cuts off exponentially, and sums over m_0 and n_0. Upon dividing by the numbers of particles $LP/\omega = L/w$ in a system of length LP, one obtains

$$\epsilon_0 = \frac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N}\Delta t_m \Delta t_n \mathcal{G}(\zeta_n - \zeta_m) \tag{4.13}$$

for the energy per particle where the subscripts of (4.9) have been omitted from m and n, and we have introduced a new function

$$\mathcal{G}(x) = w\sum_{\nu=-\infty}^{\infty}g[\frac{x+\nu}{w}] \tag{4.14}$$

which depends implicitly on both w and κ (or r). Note that

$$\mathcal{G}(x) = \mathcal{G}(1+x) = \mathcal{G}(-x) \tag{4.15}$$

is periodic and symmetrical about $x = 0$ and $x = 0.5$, and convex for x between 0 and 1, as depicted in Fig. 4.

V. FINDING THE GROUND STATE

The energy per particle ϵ_1 corresponding to H_1, (2.10), is easily evaluated when w is irrational by noting that the sequence of equally spaced points on the z axis which form the arguments of f_ω in (4.3) will eventually approach a uniform distribution if mapped modulo P into the interval $[0, P)$. That is to say, the fraction of these points falling inside an interval of type l on the z axis, which is the same as the fraction of particles whose positions lie in parabolas of type l, is equal to

$$\psi_l = \zeta_l - \zeta_{l-1}, \tag{5.1}$$

with ζ_l, (4.12), equal to $\bar{z}_l/P$. In view of (4.5),

$$\zeta_{n+N} = 1 + \zeta_n \tag{5.2}$$

and therefore

$$\sum_{l=1}^{N}\psi_l = 1. \tag{5.3}$$

As a consequence,

$$\epsilon_1 = \sum_{l=1}^{N}h_l\psi_l = -\sum_{l=1}^{N}\eta_l\zeta_l + h_1 \tag{5.4}$$

where

$$\eta_l = h_{l+1} - h_l, \tag{5.5}$$

and because the h's are periodic, (2.5),

$$\sum_{l=1}^{N}\eta_l = 0. \tag{5.6}$$

Thus the total energy per particle $\epsilon = \epsilon_0 + \epsilon_1$ can be written in the form

$$\epsilon = \frac{1}{2}\sum_{n=1}^{N}(\Delta t_n)^2 \mathcal{G}(0) + \sum_{m=1}^{N-1}\sum_{n=m+1}^{N}\Delta t_m \Delta t_n \mathcal{G}(\zeta_n - \zeta_m) - \sum_{m=1}^{N}\eta_m \zeta_m + h_1 \tag{5.7}$$

by combining (4.13), slightly rewritten using (4.15), with (5.4). Here h_1 is an additive constant which is set equal to zero in the following discussion. Then ϵ is a function of the unknown parameters $\zeta_1, \zeta_2, ..., \zeta_N$, and must be minimized by varying these parameters. In fact, adding the same constant to every ζ_n leaves ϵ unchanged (note Eq. 5.6) and therefore, since the ψ's, (5.1), cannot be negative, it suffices to consider the problem of minimizing ϵ on the *simplex*

$$0 = \zeta_0 \leq \zeta_1 \leq \zeta_2 \leq \ ... \ \leq \zeta_{N-1} \leq \zeta_N = 1. \tag{5.8}$$

One can think of the $\{\zeta_m\}$ as the positions of a set of N "quasi-particles" located on a circle of unit circumference, interacting with each other through a set of pair potentials given by $\mathcal{G}$ and, in addition, subjected to constant single-particle forces (the η's), whose sum is zero. The fact that $\mathcal{G}(x)$ has a minimum at $x = \frac{1}{2}$ means that the pair forces tend to keep the quasi-particles separated, although the imposition of suitable single-particle forces can push two or more together. However, the order (5.8) must be preserved: these quasi-particles have hard cores and will not move through each other.

Note that ϵ, regarded as a function of the ζ_j on the domain (5.8), is a sum of continuous convex functions, and is therefore continuous and convex. As a continuous function on a compact domain, it necessarily has a minimum someplace on (5.8), possibly on the boundary. Either ϵ takes its minimum at a unique point or on some larger convex subset of (5.8). If w is a rational number one can find examples where the minimum is not unique. These correspond to (first-order) phase transitions where one can have two or more distinct ground state configurations. On the other hand, if w is irrational, ϵ is a strictly convex function which achieves its minimum at a unique point in the simplex (5.8). The strict convexity of ϵ in this case arises from the strict convexity of $\mathcal{G}(x)$, whose derivative with respect to x has a dense set of discontinuities on the interval $(0, 1)$ when w is irrational.

Once the $\{\zeta_m\}$ are known, and thus the $\{\bar{z}_m\}$, see (4.12), the ground state configuration $\{u_j\}$ and the hull function f_ω, (4.3) can be obtained by means of the following construction. Define the piecewise constant and step periodic function

$$T(z) = t_m \text{ for } \bar{z}_{m-1} < z \leq \bar{z}_m, \tag{5.9}$$

see Fig. 5, so that in the ground state

$$\tau_k = T(k\omega + c). \tag{5.10}$$

Inserting this expression in (3.8) yields

$$u_j = \sum_{k=-\infty}^{\infty} g(j-k)T(k\omega + c) = \sum_{l=-\infty}^{\infty} g(l)T(j\omega + c - l\omega). \tag{5.11}$$

Comparison with (4.3) shows that

$$f_\omega^-(z) = \sum_{l=-\infty}^{\infty} g(l)T(z - l\omega), \tag{5.12}$$

where the sum yields f_ω^- because T has been defined to be continuous from the left. If at each discontinuity one sets $T(\bar{z}_m)$ equal to t_{m+1} rather than t_m, (5.12) will yield f_ω^+.

VI. CONCLUSION

We have shown how the problem of finding ground state configurations for a Frenkel-Kontorova model in a system of parabolas of identical curvature, assuming the system has a finite period, can be reduced to finding the minimum of a certain convex function, (5.7), over the variables $\{\zeta_n\}$ belonging to a finite simplex (5.8). While this second minimization problem is not trivial, the examples in our previous paper [24] show

that the solution can be worked out in particular cases with a certain amount of effort, for instance, by treating the $\{\zeta_n\}$ as parameters and computing the corresponding $\{\eta_n\}$. An efficient numerical procedure for finding the minimum, which works well for N up to the order of 200, is discussed in the paper which follows [31].

It is natural to ask whether further generalizations of this type of model might prove interesting. There are several possibilities worth considering: First, one can imagine taking the limit $N \to \infty$ with P held finite in such a way that V converges to some *smooth or piecewise smooth* periodic potential, such as a cosine. While it is unlikely that such an approach will yield an exact solution for the ground state of an arbitrary smooth periodic potential, it may nonetheless provide some interesting insights, and preliminary studies of this problem are encouraging, see [32].

Second, one can imagine a limit with both N and P tending to infinity in a way which leaves their ratio fixed, thus yielding an example of a potential, still composed of parabolas, which is *quasiperiodic* or possesses some other deterministic form of non-periodicity. An exact solution for such a case would be quite interesting.

Third, one might hope to study cases in which V consists of parabolas of two (or more) different curvatures; for example, parabolas which meet at points where their first derivatives are continuous and their second derivatives discontinuous. Such models have been studied numerically [33]. An interesting analytical investigation of a particular case and the corresponding "tent map" has been performed by Bullett [34]. The basic difficulty with non-uniform curvature is that the Green's function needed to solve the counterpart of (3.1) is much more difficult to calculate. Yet the fact that novel phenomena appear already when the basic $N = 1$ parabolic model is extended to $N = 2$ suggests that any progress in this direction would be worth the effort.

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APPENDIX A: MINIMUM DISTANCE OF APPROACH TO DIVIDING POINTS.

Aubry's theorems [30] for minimum energy and ground state configurations require that $V(u)$ be a smooth function, a condition violated at dividing points, (2.6), where the first derivative of the potential is discontinuous. This difficulty is easily circumvented by noting that, as demonstrated below, no particle in a minimum energy configuration can come closer than a minimal distance $\delta_0 > 0$ to a dividing point. Consequently one can always suppose, in order to apply Aubry's arguments, that $V(u)$ has been replaced by a smooth $\bar{V}(u)$ identical to $V(u)$ except for u closer to a dividing point than δ_0, with $\bar{V}$ always greater than or equal to V (see Fig. 6). Minimum energy configurations of $\bar{V}$ are identical to those of V, as otherwise one could lower the energy by moving a single particle, following the reasoning given below.

Assume that a dividing point occurs at $u = 0$, and that particle 1 of a minimum energy configuration falls in the parabola to the right of this point, at $u_1 = b > 0$. Ignoring an additive constant, we can write, for u near zero,

$$V(u) = \begin{cases} \kappa u^2/2 - \alpha u & \text{for } u > 0, \\ \kappa u^2/2 + (\gamma - \alpha) & \text{for } u < 0, \end{cases} \tag{A1}$$

with α a constant and $\gamma > 0$ the discontinuity in $V'(u)$ at $u = 0$.

If particles u_0 and u_2 are held fixed, the part of the energy H, (2.1), involving u_1 can be written as $\hat{V}(u_1)$, where, omitting an additive constant,

$$\hat{V}(u) = V(u) + u^2 - (u_0 + u_2)u. \tag{A2}$$

Of course $\hat{V}(u)$ must be a minimum at

$$u_1 = b = (u_0 + u_2 + \alpha)/(2 + \kappa) > 0, \tag{A3}$$

where it takes the value

$$- (u_0 + u_2 + \alpha))^2/(4 + 2\kappa). \tag{A4}$$

If b is smaller than $\gamma/(2 + \kappa)$, $\hat{V}(u)$ also has a local minimum at

$$u_1' = (u_0 + u_2 + \alpha - \gamma)/(2 + \kappa) < 0, \tag{A5}$$

where it takes the value

$$- (u_0 + u_2 + \alpha - \gamma)^2/(4 + 2\kappa). \tag{A6}$$

Now (A6) cannot be less than (A4), as otherwise the energy would be lowered by changing u_1 to u_1'. (The argument is not affected by the possible presence of another dividing point between u_0 and u_1', as in that case the energy at u_1' would be even less than (A6).) Consequently one has

$$|u_0 + u_2 + \alpha - \gamma| = |(2 + \kappa)b - \gamma| \le u_0 + u_2 + \alpha = (2 + \kappa)b, \tag{A7}$$

and thus a lower bound

$$\gamma \le 2(2 + \kappa)b \tag{A8}$$

for b. As the discontinuity γ in $V'(u)$ at the dividing point $\bar{t}_j$ is $\kappa \Delta t_j$, we conclude that no particle in a minimum energy configuration can come closer than

$$\delta_0 = [\frac{\kappa}{4 + 2\kappa}] \min_{j \epsilon \mathbb{Z}} \Delta t_j \tag{A9}$$

to one of the dividing points.

APPENDIX B: HULL FUNCTION FOR RATIONAL WINDING NUMBER

It is sufficient to consider the case in which $P = 1$ and $c = 0$, and as $w = p/q$ is fixed, the subscript ω can be omitted from the hull function f. As shown in [30], a ground state configuration $\{u_j\}$ is periodic, with

$$u_{j+q} = u_j + p \tag{B1}$$

for every j. Therefore, for any integer m, we can define

$$f(m/q) = u_j - k, \tag{B2}$$

where j and k are any two integers satisfying

$$jp - kq = m. \tag{B3}$$

The fact that p and q are relatively prime means that (B3) always has solutions, while (B1) ensures that two solutions yield the same result when inserted in (B2), and that (4.4) is satisfied with $P = 1$:

$$f(1 + z) = 1 + f(z). \tag{B4}$$

Let s and t be two integers satisfying

$$sp - tq = 1, \tag{B5}$$

and define a second ground state configuration $\{v_j\}$ by means of:

$$v_j = u_{j+s} - t. \tag{B6}$$

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Using (B2), (B5), and (B6) one finds that:

$$u_{ms} = f(\frac{m}{q}) + mt, \quad v_{ms} = f(\frac{m+1}{q}) + mt. \tag{B7}$$

A consequence of the property of "total ordering" of ground states which is proved in [30] is that if $v_j \leq u_j$ for one value of j, this must also hold for all values of j. Applied to (B7), this means that if $f[(m+1)/q]$ is less than or equal to $f(m/q)$ for one value of m, the same is true for all values of m, a result which clearly contradicts (B4). Hence

$$f(\frac{m+1}{q}) > f(\frac{m}{q}) \tag{B8}$$

for every m, and f is a strictly increasing function on the discrete set where it is defined.

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FIG. 1.   Labeling of the minima and dividing points for successive parabolas forming $V(u)$.

FIG. 2.   The function $g(x)$ for $\kappa = 0.5$.

FIG. 3.   A hull function $f_\omega(z)$ showing the relationship of the dividing points $\bar{z}_n$ and $\bar{t}_n$.

FIG. 4.   The function $\mathcal{G}(x)$ for $\kappa = 0.2$, w equal to the golden mean (0.618...).

FIG. 5.   The function $T(z)$, see text.

FIG. 6.   The smooth potential $\bar{V}(u)$, dashed curve, is identical to $V(u)$, solid curve, except near the dividing points of the latter.